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Low-energy Scattering of Positronium by Atoms

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Abstract

The survey reports theoretical studies involving positronium (Ps) - atom scattering. Investigations carried out in last few decades have been briefly reviewed in this article. A brief description of close-coupling approximation (CCA), the first-Born approximation (FBA) and the Born-Oppenheimer approximation (BOA) for Ps-Atom systems are made. The CCA codes of Ray et al [1-6] are reinvestigated using very fine mesh-points to search for resonances. The article advocates the need for an extended basis set & a systematic study using CCAs.

1 Introduction

The discovery of positronium (Ps), a hydrogen (H) like atom formed by a positron (e^+) and an electron (e^-) in 1953 by Deutsch [7], is an invaluable achievement of the modern science. The atom is itself its anti-atom. Interesting property is that its charge and mass centers coincide. The existence of Ps was first predicted by S. Mohorovicic in 1934 [8] and later on by Ruark in 1945 [9] based on their theoretical investigations which encouraged Deutsch in 1949 [10] to carry out his experimental investigation. The concept of anti-particle was introduced by Dirac in 1928 [11-12] as an anti-electron which was later experimentally observed by Anderson in 1932 [13] and was named as positron.

The collision physics is the most important area of the modern science. The most successful atomic-model by Bohr (1913) and Sommerfeld (1916) was based on the well-known Rutherford scattering (1911) experiment and theory; needless to say that the atomic concept was conceived more than a century ago by Dalton (1808), Gay-Lussac (1808), Avogadro (1811), Maxwell (1811), Mendeleef (1869) and others.

The theoretical studies on Ps and gas atom scattering was initiated by Massey and Mohr [14-15] in 1954 due to its interesting properties. The present progress is due to the continued interests of Fraser [16-18], Fraser & Kraidy [19], Hara & Fraser [20], Martin & Fraser [21], Barker & Bransden [22-23], Bransden [24], Drachman & Houston [25-26], Drachman [27-29], Au & Drachman [30], DiRienzi & Drachman [31-32], Schrader et al [33] and the realization of the fact of all the recent workers doing theories [1-6,34-51] and experiments [52-57] in different countries and different places of the world. The recent news published on 'Universe Today' dated June 8, 2005 has the headline, "The search for Positronium". This could be an important source of many new ideas leading to new physics.

The positrons and Ps are currently employed in the exploration of fundamental effects ranging from condensed matter physics to astrophysics as well as in the diagnostics of living biological systems and of the electronic and structural properties

of industrially important materials. The study of collisions of neutral positronium with other atoms (and molecules) has a number of novel features arising from its light mass and from the coincidence of its centres of charge and mass. Aside from this intrinsic interest, Ps collision data are expected to enhance our understanding of positron slowing down in dense media, Ps diffraction from surfaces, interactions of Ps injected into a plasma, etc. Various industrial applications of positron and positronium beams are discussed by Coleman [58].

Two interacting atoms mutually induce a symmetrical pair of dipoles [59]. The induced polarization potential is the same for electron-atom and positron-atom scattering, in both cases they are attractive [24]. Ps is a highly polarizable atom, its polarizability is eight times higher than that of H. They can exist in two different spin states depending on the spin of positron and electron. The singlet is known as para-Ps with a life time $\sim 10^{-10}$ s and the triplet is known as ortho-Ps having life time $\sim 10^{-7}$ s. The electrons are indistinguishable particles. Two electrons can interchange their positions, the phenomenon is known as exchange. The exchange is highly important at low incident energies in presence of more than one electron. The electron spins can be up or down. If both the spins are parallel and total spin is 1, it is known as triplet (-) state; if antiparallel, the total spin is 0 and is known as singlet (+) state.

2 Resonances

In collision physics, the existence of a resonance is an important phenomenon. When a microscopic moving object which is a wave, enters into the scattering chamber near the target, it faces interactions. When it comes out of the scattering zone, the original incident wave gathers a phase shift and the new wave is known as scattered wave. The change in phase which is named as phase shift is the parameter that carries the information of the scattering process. A rapid change in phase shift by π radian in a very narrow energy interval of the incident wave is an indication of the presence of a resonance. It indicates the existence of a bound system if in the s-wave elastic scattering and below threshold of excitation. One can calculate the width of a resonance to get the life time (τ) of the newly formed system.

It is an extremely difficult job to detect a resonance since successful identification needs (i) a very accurate calculation and (ii) sufficient computation facilities. A large number of mesh-points in a very small energy interval, generally $\sim 10^{-2} - 10^{-3}$ eV is required. It necessitates a high-speed computer with a sufficient memory, the knowledge of mathematical computation and programming languages e.g. FORTRAN.

We are interested to discuss the scattering processes at low energies. At high energies the projectile usually ignores all the important delicate interactions with target, so generally it carries no valuable information. At very low energies below excitation threshold, elastic scattering is the only real process. But from just above the threshold different excitation, ionization etc. channels start to open. It is a very difficult task to study the scattering processes at intermediate energies due to presence of many different channels and a very close-coupling among them. The total cross section is the sum of the integrated cross sections of all these channels. Besides these, the partial wave contribution from higher angular momenta start

to dominate above the threshold. Many close peaks may arise in the cross section at the intermediate energies due to opening of different channels and their mixing. These are also named as resonances and have been studied by Higgins & Burke [60-61], Sarkar et al [62-63]. However Zhou et al [64] commented against such resonances. So the subject of above threshold resonances needs more investigation. Above threshold, the phase shift becomes a complex quantity and is known as eigen phase shift.

2.1 Below threshold

The kind of resonances we are interested in, is completely different from the above threshold resonances. This type of a resonance is feasible only below threshold of first excitation when elastic cross section is the total cross section and only s-wave dominates. One needs to investigate both the phase shift and the cross section, but should be careful to use the formulation which derives the cross section directly from amplitude and not from phase shift. If it is a true resonance, this should be reflected both in phase shift and in cross section. It is actually to take a precautionary measure for successful detection since the calculation of phase shift involves a tan-inverse function which may create a numerical error.

The phase shift δ_l can be decomposed as

$$\delta_l = \xi_l + \eta_l.$$

ξ_l corresponds to the hard sphere scattering or non-resonant part; it does not depend on the shape and depth of the potential. The term η_l depends on the details of the potential. The quantities ξ_l and η_l vary, in general, slowly and smoothly with the incident particle energy. But in certain cases η_l may vary rapidly in a small energy interval of width Γ about a given energy value E_R such that we can write

$$\eta_l = \eta_l^R = \tan^{-1} \frac{\Gamma}{2(E_R - E)}$$

In that energy interval the phase shift is therefore given approximately by $\delta_l \simeq \xi_l + \eta_l^R$.

The physical significance of a narrow resonance can be inferred by examining the amplitude of the radial wave function inside the interaction region. The probability of finding the scattered particle within the potential is much higher near the resonance energy $E = E_R$, so that in that case the particle is nearly bound in the well. Thus the resonance may be considered as a metastable state whose lifetime τ , which is much longer than a typical collision time, can be related to the resonance width Γ by using the uncertainty relation $\Delta t \Delta E \geq \hbar$. Thus, with $\Delta t \simeq \tau$ and $\Delta E \simeq \Gamma$, we have $\tau \simeq \frac{\hbar}{\Gamma}$.

The shape of the cross section curve near a resonance as a function of energy depends on the non-resonant phase shift ξ_l . For the s-wave scattering it is

$$\sigma_l = \frac{\sin^2 \xi_l (E_R - E)^2 + \cos^2 \xi_l \Gamma^2 + \sin 2\xi_l (E_R - E) \Gamma / 2}{(E_R - E)^2 + \frac{\Gamma^2}{4}}$$

Two limiting cases for non-resonant phase shift are 0 and $\pi/2$. In the first case the above equation becomes

$$\sigma_l = \frac{\Gamma^2}{(E_R - E)^2 + \frac{\Gamma^2}{4}}$$

which is symmetric and represents a rise in cross section at the resonance energy. In the other case

$$\sigma_l = \frac{(E_R - E)^2}{(E_R - E)^2 + \frac{\Gamma^2}{4}}$$

which is also symmetric but goes down to zero at the resonance energy. If the non-resonant phase shift gets some other value then all sorts of forms of the cross section can occur.

Resonance in the singlet channel in positronium (Ps) and hydrogen (H) scattering was reported by many workers using different approaches [25,35,37-38,65-67]. It was first predicted by Drachman et al [25] using a Feshbach formalism with stabilization and complex rotation methods. Such a resonance using CCA schemes is reported for the first time by Ray [1-2,68-72].

3 Theory

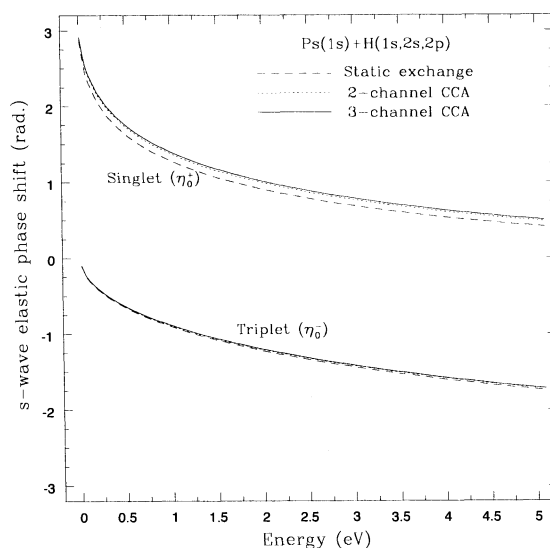


Figure 1: The s-wave elastic phase shifts below inelastic thresholds in Ps-H scattering using target-inelastic CCA theory.

3.1 Close-coupling approximation (CCA) theory

The close-coupling approximation (CCA) is a successful theory to study the low energy scattering phenomenon in atomic physics. The formulation was given by Massey [73]; he is known as the father of atomic physics. Massey applied the

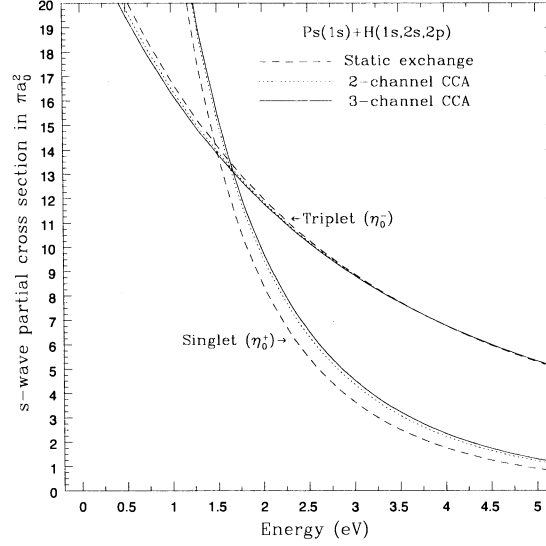


Figure 2: The s-wave elastic cross sections below inelastic thresholds in Ps-H scattering using target-inelastic CCA theory.

theory in e^- - atom scattering. Later Burke et al [74] successfully used this theory for e^+ - atom scattering. Now a days many different groups in the world are using this theory for e^-/e^+ - atom scattering. It was Fraser [16] who used it first for Ps - H scattering. Ray & Ghosh [47-48] merits the credit because they are the first who supplied detailed and converged results. They used a momentum space formalism introduced by Calcutta group [75] whereas Fraser used a coordinate space formalism to write the coupled integral equations. They again add more channels in the CCA basis [1-6,68-72,76-78]. The studies of Fraser [16-18], Fraser et al [19], Hara et al [20] were confined to static-exchange model i.e. considering only the elastic channel in the basis and the H and He targets. Ray [4-6] extended the CCA theory in Ps and lithium (Li) scattering using the static-exchange and a two-channel CCA models.

The theory is based on the very basic principle of quantum mechanics i.e. the eigen state expansion (ESE) methodology in which the total wave function of a quantum mechanical system is expressed as a linear combination of all possible states known as basis set. So one has to use a wide channel space, but practically it is not possible. The number of unknowns exceed the number of equations when non-spherical orbitals like p- and d- states of an atom are considered in channel space. So arose the necessity of an approximation. We should conserve the total angular momentum quantum numbers e.g. 'J' and 'M'. It makes the equations closed i.e. the number of unknowns are equal to the number of equations. This is known as CCA. The accuracy of the method depends on the choice of basis set.

The total wavefunction of Ps-H system Ψ^\pm satisfying the Schrödinger equation:

$$H\Psi^\pm(\mathbf{r}_p, \mathbf{r}_1, \mathbf{r}_2) = E\Psi^\pm(\mathbf{r}_p, \mathbf{r}_1, \mathbf{r}_2) \quad (1)$$

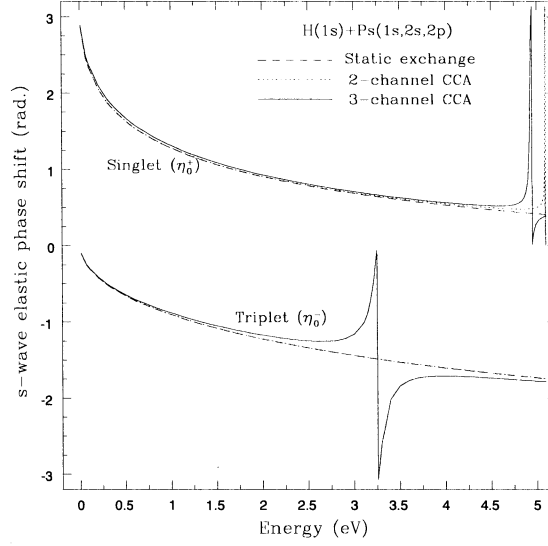


Figure 3: The s-wave elastic phase shifts below inelastic thresholds in Ps-H scattering using projectile-inelastic CCA theory.

is expressed as

$$\Psi^{\pm}(\mathbf{r}_p, \mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(1 \pm P_{12}) \sum_{n_t l_t n_p l_p L J_1 J M} \frac{F_{\Gamma_0 n_t l_t n_p l_p L J_1 J M}(\mathbf{k}, \mathbf{k}', R_1)}{R_1} \frac{U_{n_t l_t}(r_2)}{r_2} \frac{V_{n_p l_p}(\rho_1)}{\rho_1} \sum_{m_t m_p M_L} \begin{pmatrix} L & l_p & J_1 \\ M & m_p & M_1 \end{pmatrix} \begin{pmatrix} J_1 & l_t & J \\ M_1 & m_t & M \end{pmatrix} Y_{L M_L}(\hat{\mathbf{R}}_1) Y_{l_p m_p}(\hat{\rho}_1) Y_{l_t m_t}(\hat{\mathbf{r}}_2) \quad (2)$$

with

$$H = -\frac{1}{2}\nabla_p^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{|\mathbf{r}_p|} - \frac{1}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{r}_2|} - \frac{1}{|\mathbf{r}_p - \mathbf{r}_1|} - \frac{1}{|\mathbf{r}_p - \mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (3)$$

Here P_{12} stands for the exchange operator and $\mathbf{R}_i = \frac{1}{2}(\mathbf{r}_p + \mathbf{r}_i)$ and $\rho_i = \mathbf{r}_p - \mathbf{r}_i$; $i=1,2$; \mathbf{r}_1 and \mathbf{r}_2 are the position vectors of the electrons belonging to Ps and H respectively and \mathbf{r}_p , is that of the positron with respect to the center of mass of the system. $U_{n_t l_t}(\mathbf{r})/r$ and $V_{n_p l_p}(\rho)/\rho$ are the radial parts of the wavefunctions of H and Ps respectively and $F_{\Gamma_0 \Gamma}(\mathbf{k}, \mathbf{k}', R)/R$ is the radial part of the continuum wave function of the moving Ps atom; Γ_0 indicates all the quantities $n_t l_t n_p l_p L J_1 J M$ of Γ at the initial channel.

Projecting the Schrödinger Eqn.(1) just like the Hartree-Fock variational approach and integrating over the desired coordinates, we can get a set of integro-differential equations which can be transformed into the integral equations like Lippmann-Schwinger applying the asymptotic boundary conditions. These coupled integral equations can be formed either in momentum space or in configuration space. We have used momentum space formalism [75]. The set of coupled integral equations obtained for the scattering amplitudes are as follows:

$$f_{n' l', n l}^{\pm}(\mathbf{k}', \mathbf{k}) = B_{n' l', n l}^{\pm}(\mathbf{k}', \mathbf{k}) + \frac{1}{2\pi^2} \sum_{n'' l''} \int d\mathbf{k}'' \frac{B_{n' l', n'' l''}^{\pm}(\mathbf{k}', \mathbf{k}'') f_{n'' l'', n l}^{\pm}(\mathbf{k}'', \mathbf{k})}{k''^2 - k_{n'' l''}^2 + i\epsilon} \quad (4)$$

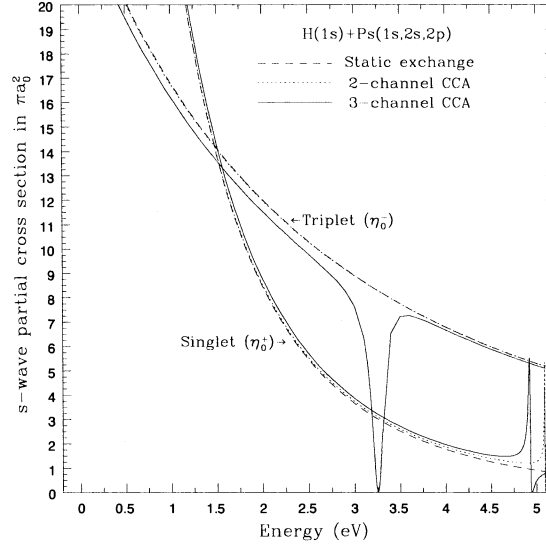


Figure 4: The s-wave elastic cross sections below inelastic thresholds in Ps-H scattering using projectile-inelastic CCA theory.

B^\pm indicate the Born-Oppenheimer [79] scattering amplitudes, plus(+) is for the singlet channel and minus(-) for triplet channel. The formulation for the FBA and BOA matrix elements are discussed [80-86] and briefly described here. Similarly f^\pm indicate the unknown scattering amplitudes for the singlet and the triplet channels respectively. The summation over $n''l''$ is to include various channels.

These three dimensional coupled integral equations involving $f_{n'l',nl}(\mathbf{k}', \mathbf{k})$ and $B_{n'l',nl}(\mathbf{k}', \mathbf{k})$ can be reduced to the corresponding one dimensional forms through partial wave analysis using the expansion like:

$$\tau_{n'l'm',nlm}^\pm(\mathbf{k}', \mathbf{k}) = (kk')^{-1/2} \sum_{J,M} \sum_{L,M_L} \sum_{L',M'_L} \sum_{J_1,M_1} \sum_{J'_1,M'_1} \langle L'l'_p, M'_L m'_p | J'_1 M'_1 \rangle$$

$$\langle L l_p, M_L m_p | J_1 M_1 \rangle \langle J'_1 l'_t, M'_1 m'_t | J M \rangle \langle J_1 l_t, M_1 m_t | J M \rangle$$

$$Y_{L'M_L'}(\hat{\mathbf{k}}') Y_{LM_L}(\hat{\mathbf{k}}) \tau^{J\pm}(k' n'_p n'_t l'_p l'_t, k n_p n_t l_p l_t) \quad (5)$$

The resulting one dimensional coupled integral equations can be written as a matrix equation like

$$[\mathbf{A}]_{N \times N} [\mathbf{X}]_{N \times 1} = [\mathbf{B}]_{N \times 1} \quad (6)$$

which can be solved by matrix inversion method. Here $[\mathbf{A}]$ is the scattering matrix of $N \times N$ type formed by Born and Born-Oppenheimer scattering amplitudes, $[\mathbf{X}]$ is the column matrix of $N \times 1$ type formed by unknown CCA scattering amplitudes and $[\mathbf{B}]$ is again a column matrix of $N \times 1$ type formed by the Born and Born-Oppenheimer [79] scattering amplitudes; the dimension(N) depends on the number of channels included in the expansion basis. We have calculated all the Born and Born-Oppenheimer amplitudes exactly following an analytic approach and then

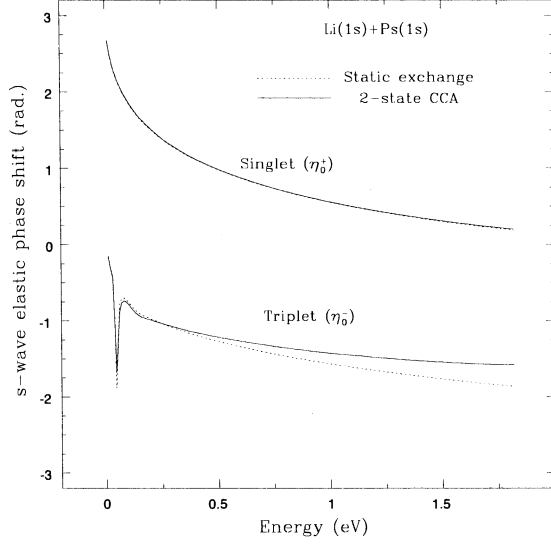


Figure 5: The s-wave elastic phase shifts below inelastic thresholds in Ps-Li scattering using target-inelastic CCA theory.

the remaining part is carried out following numerical approach using computer and FORTRAN programming. The two sets of one dimensional coupled integral equations of scattering amplitudes in momentum space for the singlet(+) and triplet(-) channels respectively, are solved separately for each partial wave(L).

We employ different projectile-elastic and projectile-inelastic CCA-schemes to investigate Ps-H and Ps-Li scattering in the energy region below inelastic threshold. We study s-wave elastic phase shifts and s-wave elastic cross sections using a very fine mesh-points. We perform exact calculations for all the direct and exchange matrix elements considering all the possible Coulomb interactions where the direct first-Born amplitudes vanish if the parity of Ps remains unaltered.

3.2 First-Born approximation (FBA)

The FBA amplitude for the scattering of the Ps by atomic target is expressed as,

$$F_{fi}^{B1} = -\frac{\mu}{2\pi} \int e^{-i\mathbf{k}_f \cdot (\mathbf{x} + \mathbf{r}_1/2)} \eta_f^*(|\mathbf{x} - \mathbf{r}_1|) \phi_f^*(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) [V_{int}] \phi_i(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \eta_i(|\mathbf{x} - \mathbf{r}_1|) e^{i\mathbf{k}_i \cdot (\mathbf{x} + \mathbf{r}_1/2)} d\mathbf{x} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \dots d\mathbf{r}_N \quad (7)$$

where μ is the reduced mass of the system; \mathbf{x} , \mathbf{r}_1 and \mathbf{r}_i are the position vectors for the positron, the electron in the Ps and the i -th electron in the target atomic system respectively w.r.t. center of mass of the system. N is the number of active electrons present in the system. η_i and η_f are respectively the initial and final state wavefunctions for the positronium atom whereas ϕ_i and ϕ_f are the initial and final state wavefunctions of the atomic target. V_{int} is the interaction potential due to electrostatic Coulomb interaction between the two atomic systems and is

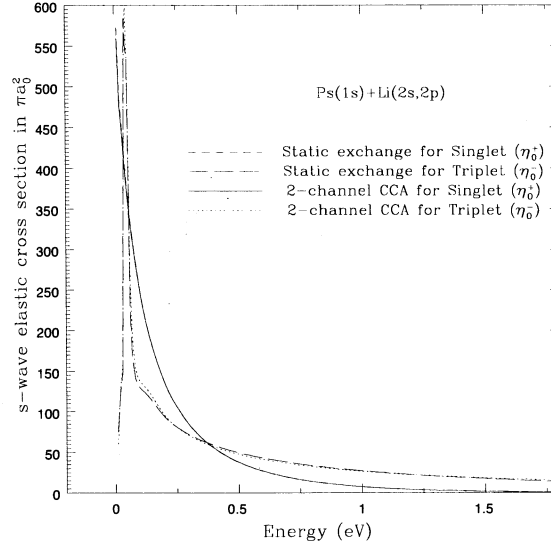


Figure 6: The s-wave elastic cross sections below inelastic thresholds in Ps-Li scattering using target-inelastic CCA theory.

given by

$$V_{int} = \frac{Z}{x} - \frac{Z}{r_1} - \sum_{i=2}^N \frac{1}{|\mathbf{x} - \mathbf{r}_i|} + \sum_{i=2}^N \frac{1}{|\mathbf{r}_1 - \mathbf{r}_i|} \quad (8)$$

Making the substitution $\boldsymbol{\rho} = \mathbf{x} - \mathbf{r}_1$ and $\mathbf{R} = (\mathbf{x} + \mathbf{r}_1)/2$ and performing the integrations, the above scattering amplitudes reduce to a general form like :

$$F_{fi}^{B1} = -\frac{4}{q^2} \{I_{Ps}\} \{I_{target}\} \quad (9)$$

Here $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$, is the momentum transfer; \mathbf{k}_i and \mathbf{k}_f are the momenta of the projectile in the initial and final states respectively. I_{Ps} and I_{target} , the form factors for Ps and target respectively are given by

$$I_{Ps} = \int \eta_f^*(\boldsymbol{\rho}) \{e^{-i\mathbf{q} \cdot \boldsymbol{\rho}/2} - e^{i\mathbf{q} \cdot \boldsymbol{\rho}/2}\} \eta_i(\boldsymbol{\rho}) d\boldsymbol{\rho} \quad (10)$$

and

$$I_{target} = \int \phi_f^*(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) [Z - \sum_{i=2}^N e^{i\mathbf{q} \cdot \mathbf{r}_i}] \phi_i(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \prod_{i=2}^N d\mathbf{r}_i \quad (11)$$

Here Z represent the nuclear charge of target atom.

3.3 Born-Oppenheimer approximation (BOA)

The differential cross section in Ps-H scattering is defined as

$$\frac{d\sigma}{d\hat{\mathbf{k}}_f} = \frac{k_f}{k_i} \left\{ \frac{1}{4} |F + G|^2 + \frac{3}{4} |F - G|^2 \right\} \quad (12)$$

if F and G are respectively the direct and exchange matrix elements in space part only.

Accordingly the integrated or the total cross section (σ) can be defined as:

$$\sigma(E_i) = \frac{k_f}{k_i} \int d\hat{\mathbf{k}}_f \left[\frac{1}{4} |F(\hat{\mathbf{k}}_f) + G(\hat{\mathbf{k}}_f)|^2 + \frac{3}{4} |F(\hat{\mathbf{k}}_f) - G(\hat{\mathbf{k}}_f)|^2 \right] \quad (13)$$

Where

$$F(\hat{\mathbf{k}}_f) = -\frac{1}{\pi} \int e^{-i\mathbf{k}_f \cdot \mathbf{R}_1} \eta_f^*(\boldsymbol{\rho}_1) \Phi_f^*\{\mathbf{r}_2\} [V_{int}^F] e^{i\mathbf{k}_i \cdot \mathbf{R}_1} \eta_i(\boldsymbol{\rho}_1) \Phi_i\{\mathbf{r}_2\} d\mathbf{x} d\mathbf{r}_1 d\mathbf{r}_2 \quad (14)$$

$$G(\hat{\mathbf{k}}_f) = -\frac{1}{\pi} \int e^{-i\mathbf{k}_f \cdot \mathbf{R}_2} \eta_f^*(\boldsymbol{\rho}_2) \Phi_f^*\{\mathbf{r}_1\} [V_{int}^G] e^{i\mathbf{k}_i \cdot \mathbf{R}_1} \eta_i(\boldsymbol{\rho}_1) \Phi_i\{\mathbf{r}_2\} d\mathbf{x} d\mathbf{r}_1 d\mathbf{r}_2 \quad (15)$$

with $\mathbf{R}_j = \frac{1}{2}(\mathbf{x} + \mathbf{r}_j)$ and $\boldsymbol{\rho}_j = (\mathbf{x} - \mathbf{r}_j)$; $j=1,2$. Here, \mathbf{x} is the coordinate of positron in Ps, and \mathbf{r}_j ; $j=1,2$ are that of electrons in Ps and in H respectively in the incident channel w.r.t. the center of mass of the system. Functions η and Φ indicate the wave functions of Ps and H. Subscript 'i' identifies the incident channel, whereas 'f' represents the final channel. Accordingly \mathbf{k}_i and \mathbf{k}_f are the momenta of the projectile in the initial and final channels respectively.

$$V_{int}^F = \frac{1}{|\mathbf{x}|} - \frac{1}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{x} - \mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (16)$$

$$V_{int}^G = \frac{1}{|\mathbf{x}|} - \frac{1}{|\mathbf{r}_2|} - \frac{1}{|\mathbf{x} - \mathbf{r}_1|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (17)$$

Indices F and G indicate the direct and exchange channels respectively.

The computation of Born-exchange matrix element is much more difficult than the direct Born-element. The Fourier transform

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{p^2 + \lambda^2} d\mathbf{p},$$

the Bethe integral

$$\int \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{r} d\mathbf{r} = \frac{4\pi}{k^2}$$

and the properties of Dirac δ -function are mainly used for analytical evaluation. The numerical integrations are carried out using Gauss-Legendre quadratures.

4 Results & discussion

In the present review article, we discuss the elastic scattering at low energies below the inelastic threshold of excitation in Ps-H and Ps-Li scattering. We use different target-inelastic and projectile-inelastic CCA schemes to study s-wave elastic phase shifts and s-wave elastic cross sections with a very fine mesh points to search for resonances. The incident energies are chosen from 0 to 5.1 eV for Ps-H system. Our results using the static-exchange approximation, target-inelastic 2-channel and 3-channel CCAs are presented in figures 1 & 2 and are giving no trace of resonances. But both the phase shifts and cross sections using projectile-inelastic 2-channel and 3-channel CCAs are showing perfect resonances in singlet channel and are presented in figures 3 & 4. The singlet resonance using projectile-inelastic

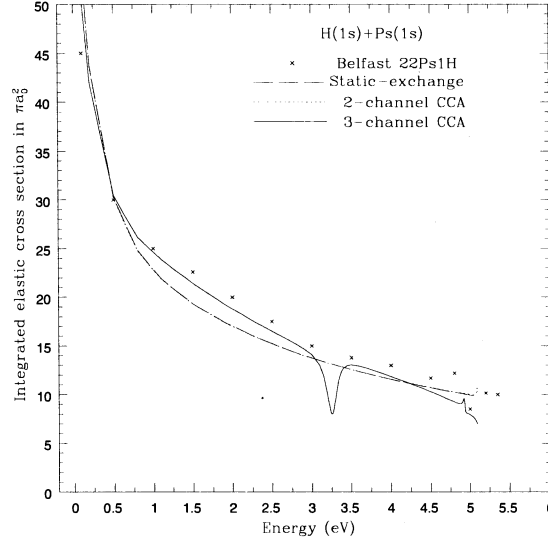


Figure 7: Comparison of total cross sections for Ps-H scattering below inelastic thresholds using projectile-inelastic CCAs, static-exchange approximation and 22Ps1H coupled-pseudostate R-matrix theory.

3-channel CCA is shifted to lower energies and broadened in width than 2-channel CCA when it was very close to first excitation threshold. All the corresponding triplet results are also presented in the same figures 1 to 4. No triplet resonance is found except using the projectile-inelastic 3-channel CCA scheme. The triplet resonance is found near the energy 3.25 eV. The corresponding s-wave partial cross section is giving a sharp well. All resonances satisfy the Breit-Wigner formulation of cross section. This kind of perfect resonances were first time observed by Ray [1-2,68-72] using different projectile-inelastic CCA schemes. The singlet resonance was predicted earlier [25,35,46,66-67], but the triplet was new.

We also reinvestigate the s-wave elastic phase shifts and cross sections below inelastic threshold for Ps-Li scattering using static-exchange approximation and 2-channel target-inelastic CCA in a similar fashion. Energy region is chosen from 0 to 1.8 eV i.e. below inelastic threshold of first excitation. Our findings are presented in figures 5 & 6 and are very similar to the earlier results. The triplet channel is more sensitive to long-range forces due to dipole polarizability near to threshold. This long range dynamic effect [87-88] is introduced into our calculation through Li(2p) state. In a different way, it is the quantum mechanical effect of strong coupling between the Li(2s) and Li(2p) states. There is no trace of resonances in the singlet channel using both the CCA schemes. But the triplet channel is showing a rapid change in phase shifts $\sim \pi/2$ radian in both the static-exchange and 2-channel CCA at very close to zero energy and the corresponding partial wave cross sections are showing sharp peaks. However these are not resonances. The definition of below-threshold resonances admits a phase shift change of π radian. It is not known to us what it indicates.

In figure 7, we compare the total cross sections. These are again the total elastic cross sections since at the energy region below inelastic/excitation threshold

elastic channel is the only open channel. The projectile-inelastic 2-channel and 3-channel CCA cross sections are presented with static-exchange approximation [47-48] and the 22Ps1H coupled-pseudostate R-matrix data of Blackwood et al [37]. The present results show good agreement. The well in the total cross section curve using projectile-inelastic 3-channel CCA supports the triplet resonance. The small peaks using projectile-inelastic 2-channel and 3-channel CCAs are supporting the singlet resonance.

In addition, the present triplet phase shift data for Ps-H scattering using projectile-inelastic 3-channel CCA fit nicely with non-resonant part as

$$\xi_0 = -1.4053 + 0.1295E - 0.04613E^2$$

and provides the width $\Gamma = 0.15173eV$ and resonance position $E_R = 3.2630eV$.

5 Conclusion

A brief survey on Ps-atom scattering is made. Resonances below excitation threshold are discussed. Thorough reinvestigations are made in Ps-H system with static-exchange, target-inelastic and projectile-inelastic 2-channel and 3-channel CCAs using a very fine mesh points to search for resonances. No resonance is found with static-exchange approximation and target inelastic 2-channel and 3-channel CCAs in Ps-H system. A singlet resonance found in both projectile-inelastic 2-channel and 3-channel CCAs in Ps-H system which for the first time is detected using close-coupling approximation schemes, agree well with earlier predictions. A triplet resonance with 3-channel projectile-inelastic CCA in Ps-H system is a new addition. It needs more investigations using an extended basis set and a systematic study to realize the physical cause of it. In Ps-Li system no resonance is found below inelastic threshold using both the static-exchange and target-inelastic 2-channel CCA. The comparison of total cross section curves below inelastic threshold in Ps-H system supports the existence of both the singlet and triplet resonances.

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